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Separation Science and Technology
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713708471

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Online publication date: 29 May 2002

To cite this Article Silva, E. A. Borges da , de Souza, A. A. Ulson , Guelli, S. M. A. and Souza, U.(2002) 'The use of simulated moving bed in chromatographic separation: study of the SMB configuration', Separation Science and Technology, 37: 7, 1489 — 1504
To link to this Article: DOI: 10.1081/SS-120002733
URL: http://dx.doi.org/10.1081/SS-120002733

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SEPARATION SCIENCE AND TECHNOLOGY, 37(7), 1489–1504 (2002)

THE USE OF SIMULATED MOVING BED IN CHROMATOGRAPHIC SEPARATION: STUDY OF THE SMB CONFIGURATION

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ABSTRACT

The simulated moving bed (SMB) unit in a chromatographic separation of enantiomers has been modeled and simulated by a computational program. The mathematical model of the unit considers the plug flow model with axial dispersion for the fluid phase and the linear driving force approximation for the intraparticle mass transfer rate. The model assumes the switching of the inlet and outlet streams of the unit for each time interval, and then, allows accompanying the evolution of the internal profiles of enantiomer concentration for the transient operation of the SMB. The mathematical equations with the respective boundary and initial conditions are numerically solved by finite volume method. The influence of bed configuration on the SMB performance has been studied using a computational program.

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However the purity and recovery of some species are slightly affected by configuration.

Key Words: Simulated moving bed; Configuration; Modeling; Numerical simulation

INTRODUCTION

The simulated moving bed (SMB) technology appeared as an alternative process for continuous countercurrent adsorption without the need of the solid phase movement. This operation permits to reach high efficiency, so nowadays great part of the industrial application and research in this area choose this technology, mainly when it is aimed to recover products of high aggregated value with low separation factors.

By 1961, when the conception of the SMB became well known, its application was limited to some separations developed by UOP (Universal Oil Products), called SORBEX processes (1,2). In these processes the movement of the solid was simulated through a rotary valve that periodically exchanged the inlet and outlet streams along a fixed-bed adsorber.

On this last decade, the study and the use of this technology was intensified in new areas, such as fine chemistry, pharmaceutical, biotechnology and cosmetics, and perfumes industries.

One of the most recent applications of the SMB technology is related to the separation of chiral chemical species. The separation of enantiomers is an important point, particularly in the field related to health. It is known that the optical isomers may exhibit completely different and even opposed, therapeutic values, and for this reason they are of great interest to pharmaceutical companies in the separation of isomers and enantiomers for the development of new drugs (3).

When low separation factors are involved, it is difficult to obtain a pure composition of enantiomers for conventional techniques, as the batch chromatography, and therefore, the continuous chromatography in SMB appears as a promising technique for industrial production of optical isomers. The warranty of more efficient use of the adsorbent, the supply of more concentrated species and being a fast continuous process are still three of the main advantages of the SMB unit (4). One of the inconveniences pointed by Zhong and Guiochon (4) in the application of this technology in the pharmaceutical industries would be the degree of complexity of the design, operation, and optimization of the SMB.

It is important to note that, with this new application, it caused a change in the physical configuration of an industrial unit of SMB, as shown in Fig. 1, that is, a set of fixed beds connected in series segmented by valves and inlet and outlet lines, with four sections (5).

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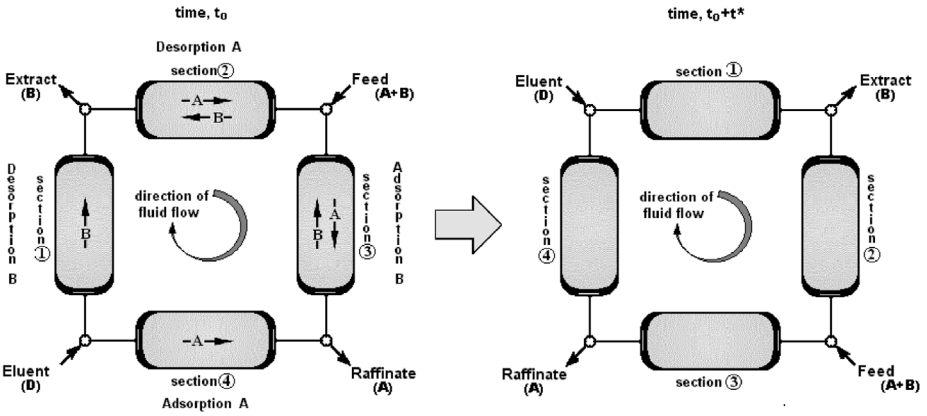

Figure 1. Simulated Moving Bed Unit—Representative scheme of the collect and admission streams switching in the unit (t^*, switching time). Functions and restrictions of species flows in the four sections of the SMB unit.

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In the system shown in Fig. 1, the fluid phase circulates through a number of fixed-bed columns, called subsections, packed with the adsorbent solid. The countercurrent operation, leading to the high mass transfer driving forces, is accomplished for the simultaneous movement in the unit of the inlet—feed and eluent—and of the outlet—raffinate and extract—streams, in fixed time intervals, called switching time, in the fluid phase flow direction. The unit is then divided into four sections, although there are other kinds of SMB units for some particular cases (6,7), each one carrying out a specific function in the separation process (each section can have many subsections). The Section 1 regenerates the adsorbent by desorption of the more strongly adsorbed species (species B); in the Section 2 and in the Section 3 occurs desorption of the less retained species (species A) and adsorption of the species B, respectively; and, finally, the Section 4, that regenerates the eluent for the adsorption of the species A.

The success of the separations by SMB chromatography depends strongly on two aspects (8): correct choice of the stationary phase and of the eluent, and the correct choice of the operation conditions. As for the second aspect mentioned, due to its complex physical configuration, the experimentation in laboratory can be a complicated task. Many techniques have been proposed to get appropriated operation conditions for the simulated moving bed. These techniques refer to the modeling and simulation tools of the phenomena and processes involved. These tools are quite attractive and are very important for the cost and time economy as well as to obtain the parameters for which the maximum unit performance is reached (9).

In order to design appropriate SMB operating conditions which maximize the unit performance, the most studied operation variables have been inlet and outlet flow rates, switching time, and number or length of subsections (10,11). The unit configuration has not been studied yet. Ching et al. (12) examined the effect of varying the system configuration in the glucose and frutose separation, and they verified that the process performance is affected slightly by the configuration in a SMB with 12 subsections. Pais et al. (13) also studied the configuration effect on performance and verified only little differences in the performance parameters—purity and recovery—among the configurations of SMB with eight subsections employed. But in spite of being slight, the differences exist, and it is interesting to dominate this operational condition, because sometimes the increase of 1% in the purity or recovery of a certain species may give an operational economy related to solvent and adsorbent consumption (14).

The objective of this work is the development of the numerical solution of a transient model of the SMB chromatography, and the study of the unit behavior and performance, analyzing some aspects related to the configuration of the subsections in a SMB with four sections.

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MODELING OF THE SMB

In general, the modeling on a SMB unit may be grouped into two categories: those represented by the true SMB configuration, where the boundary conditions in the subsections are changed periodically, and those represented by the equivalent True Moving Bed (TMB) configuration. These two modeling strategies may be treated in agreement with the equilibrium theory (9,15) or for the inclusion of a rate expression adapted to describe the mass transfer resistance (7,13,16). In the latter, the mass transfer resistances are considered in the intraparticle mass transfer rate equation, very commonly described by a linear driving force mechanism, approximation LDF. Recently Azevedo and Rodrigues (17,18) have used a bi-linear driving force mechanism (approximation Bi-LDF) to describe the intraparticle diffusion. In spite of some studies (19,20) show that in general the TMB approach has reasonable accuracy to provide an adequate representation of the SMB behavior, and it requires lower computational time, in this work it is used the SMB model for giving some more detailed information on the process dynamics.

Transient Mathematical Model

The governing equations for the transient SMB mathematical model consider the continuous fluid flow with axial dispersion for the bulk fluid phase

and the linear driving force mechanism to describe the intraparticle mass transfer rate. This mathematical model is still based on the following assumptions:

i. the process is isotherm;
ii. the fluid flow inside columns is described by axial dispersed plug flow. So, the velocities along a SMB section are constant;
iii. the "dead volumes" at both ends of the packed adsorbents are negligible, as discussed by Lu and Ching (21); and
iv. the adsorbent phase is homogeneous, so that the bed porosity (ϵ) can be considered constant along the SMB columns.

In agreement with the considerations above, the mass balance equations for the species i in a subsection k of the SMB are:

Fluid-phase mass balances in a volume element of the subsection k

$$\frac{\partial c_{ik}}{\partial t} + \frac{(1-\epsilon)}{\epsilon}\frac{\partial q_{ik}}{\partial t} + v_k \frac{\partial c_{ik}}{\partial z} - D_{ak}\frac{\partial^2 c_{ik}}{\partial z^2} = 0 \tag{1}$$

Particle mass balances

$$\frac{\partial q_{ik}}{\partial t} = k_T(q_{ik}^* - q_{ik}) \tag{2}$$

Initial conditions:

$$t = 0: \quad c_{ik} = q_{ik} = 0 \tag{3}$$

Boundary conditions:

$$z = 0, \quad t > 0: \quad c_{ik,o} = c_{ik} - \frac{D_{ak}}{v_k}\left.\frac{\partial c_{ik}}{\partial z}\right|_{z=0}, \tag{4a}$$

$$z = \mathrm{L}, \quad t > 0: \quad \left.\frac{\partial c_{ik}}{\partial z}\right|_{z=L} = 0 \tag{4b}$$

The boundary conditions depend on the section of the fixed bed column in the system. The mass balances at the nodes of the simulated moving bed identify the considered sections, in a time interval. These balances should be used in the boundary condition given by Eq. (4a), in agreement with the location of the considered column (k).

For columns inside of a section and for the extract and raffinate nodes:

$$c_{ik+1,0} = c_{ik} \tag{5a}$$

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For the eluent node:

$$c_{ik+1,0} = (v_4/v_1)c_{ik} \tag{5b}$$

For the feed node:

$$c_{ik+1,0} = (v_f/v_3)c_{if} + (v_2/v_3)c_{ik} \tag{5c}$$

These equations characterize the dependence of the boundary conditions related to time in the system. In the above-mentioned equations, c_{ik} and q_{ik} are the concentrations of the species i in the column k in the fluid phase and adsorbent phase, respectively, v_k is the fluid velocity in the column k, D_{ak} is the axial dispersion coefficient in the column k and k_T is the intraparticle mass transfer coefficient. Some kind of adsorption equilibrium isotherm (q_{ik}^*) should be used in the model.

Process Performance Parameters

The SMB performance for the separation of the binary mixture—A (less adsorbed species) and B (more retained species)—is evaluated according to Lu and Ching (21):

(a) Purity of the products in their enriched streams

$$Pu_{ra} = \frac{\int_0^{t^*} c_A dt}{\int_0^{t^*} (c_A + c_B) dt} \quad \text{(raffinate)};$$

$$Pu_{ex} = \frac{\int_0^{t^*} c_B dt}{\int_0^{t^*} (c_A + c_B) dt} \quad \text{(extract)} \tag{6}$$

(b) Recovery of the products in their enriched streams

$$Re_{ra} = \frac{Q_{ra}}{Q_f c_{Af}} \frac{\int_0^{t^*} c_A dt}{t^*} \quad \text{(raffinate)};$$

$$Re_{ex} = \frac{Q_{ex}}{Q_f c_{Bf}} \frac{\int_0^{t^*} c_B dt}{t^*} \quad \text{(extract)} \tag{7}$$

SIMULATION RESULTS

The simulation of the continuous chromatographic separation of the racemic mixture of (±)1a,2,7,7a-tetrahydro-3-methoxy-naphta-(2,3b)-oxirane—

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a chiral epoxide—in a SMB unit is accomplished. In this separation, the stationary adsorbent phase and the eluent used are, respectively, cellulose triacetate, and methanol. This system has been studied by Nicoud et al. (22), Rodrigues et al. (10,23), Pais et al. (24) and Lu and Ching (21).

The mathematical model is used to predict the behavior, in the cyclic steady state, of an SMB unit in this enantiomers separation process, and to study the effect of the unit configuration on the separation performance by the variables: purity and recovery of the species. The operation conditions and other necessary parameters to the simulation are described in Table 1, according to Lu and Ching (21). The SMB chromatography unit used in this process is composed of 12 columns packed with cellulose triacetate, each of 11 cm length and 26 mm diameter.

The concentrations of the species in the adsorbent phase, in equilibrium with the concentrations in the fluid phase, are obtained through the adsorption equilibrium isotherms given by (10):

$$q_A^* = 1.57C_A + \frac{0.261C_A}{1 + 0.045C_A + 0.127C_B} \tag{8a}$$

$$q_B^* = 1.57C_B + \frac{0.7366C_B}{1 + 0.045C_A + 0.127C_B} \tag{8b}$$

where subscript B represents the more adsorbed enantiomer, and the subscript A the less adsorbed enantiomer.

The transient mathematical model equations were numerically resolved using a computational program, developed in FORTRAN language, based on the Method of Finite Volumes, applying the interpolation functions WUDS (25). The algebraic equations systems generated by the discretization method were

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Table 1. Operation Conditions and Model Parameters in the Separation of the Chiral Epoxide in a SMB Unit

Operation Conditions		Parameters	
C_{Af}	5.0 mg/mL	Mass transfer coefficient (k_T)	6.0 min^{-1}
C_{Bf}	5.0 mg/mL	Axial dispersion coefficient(D_a)	0.129 cm^2/min
Q_f (feed)	1.52 mL/min		
Q_d (eluent)	4.53 ml/min	Number of columns	12 (3-3-3-3)
Q_{ra} (raffinate)	2.05 mL/min	Length (L)	11.0 cm
Q_{ex} (extract)	4.00 mL/min	Diameter	2.6 cm
$Q_{Recycled}$	20.37 mL/min	Bed Porosity(ϵ)	0.4
t^*	248 sec		

resolved by the Modified Strongly Implicit Method (26). The computational grid used in the simulations was 100×10 with time integration step size of 1 sec.

Considering the adopted boundary conditions, the cyclic steady state is reached by this system after 10–15 cycles, which means about 4 hr of CPU time in the Pentium II 400 MHz. A cycle is computed when a fluid stream, after having exchanged once, comes back to its initial position. Since the boundary conditions are variable with the time in the transient mathematical model, the choice of the integration time interval parameter can be fundamental in obtaining a larger precision of the numerical results. In this case, other integration time step values were tested, and taking into account the result precision and the CPU time spent, the time of 1 sec was chosen.

Results Analysis

Figure 2 shows the concentration profiles of the enantiomers in the raffinate and extract streams, in the transient state, as a function of the cycles number. In this figure, it is verified the beginning of the cyclic steady state for the system in study. The concentration value used in this transient representation is that collected in the half of the switch time interval-instantaneous concentration.

Figure 3 shows the concentration profiles of the species in the respective enriched streams for SMB operated in the first five cycles. The prediction is accomplished by the three ways of unit behavior description: the exact evolution of the concentration profiles, the average concentration profile and the instantaneous concentration (in this case, evaluated in the half of the switch time interval).

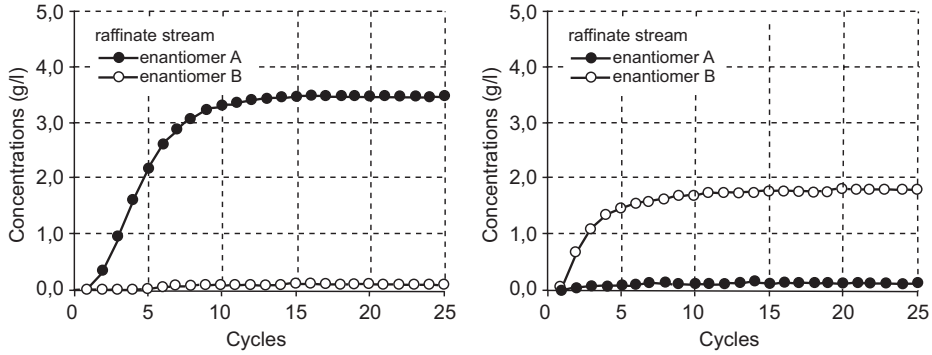

Figure 2. Evolution of the enantiomer concentration in the raffinate and extract streams with the elapsed cycles.

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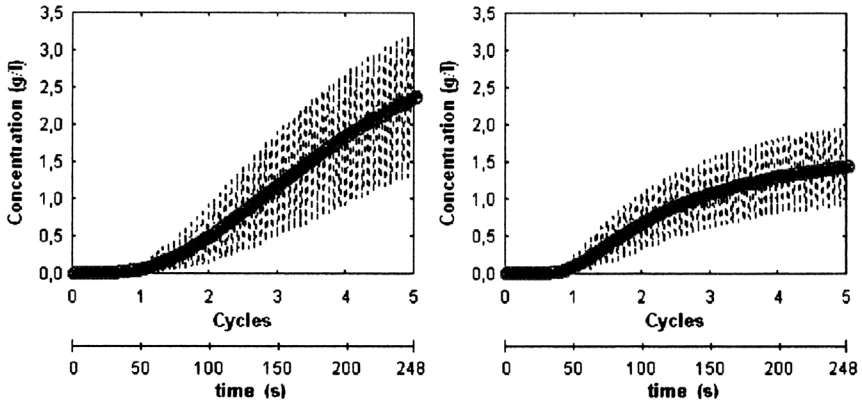

Figure 3. Concentration profiles of the enantiomers in the SMB unit with 12 subsections; (a) enantiomer less adsorbed in the raffinate stream, (b) enantiomer more adsorbed in the extract stream; (- - -) exact transient concentration profile in the unit, (⊖) average concentration profile in the switch interval, (✳) instantaneous concentration profile in the half of the switch interval.

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In Fig. 3 it is possible to verify the variation of enantiomers concentrations inside of a values range during the switching time. The width of this concentration variation within the switch interval is a function of the flow switching requirements and it decreases with the increase of the subsections number (19,20). This transient profile approaches to a line as the number of subsections tends to infinity. It is possible to obtain the concentration profile identical to the TMB unit in the characteristic steady state. In this case, the average and instantaneous concentration profiles in the unit appear quite close due to the high number of subsections involved.

The experimental and numerical instantaneous concentration profiles for the two species in the unit, at the mid-time of the switch interval, after reaching the cyclic steady state of this system, are shown in Fig. 4. The experimental results were obtained by Nicoud et al. (22).

Analyzing Fig. 4, although the values show some scatter, thus the agreement is not quantitatively accurate, but it is evident that the numerical results provide a satisfactory representation of the SMB behavior. In this figure the profiles predicted by Lu and Ching (21) are still presented. They used the intermittent moving bed model and solved it by the Method of Orthogonal Collocation in finite elements. It is possible to verify a good agreement among the numerical concentration profiles of both enantiomers. The deviations observed among the numerical and experimental values in the Section 3 were justified by Lu and Ching (21) due to the omission to the dead volume at both ends of the columns, the use of the linear driving force mass

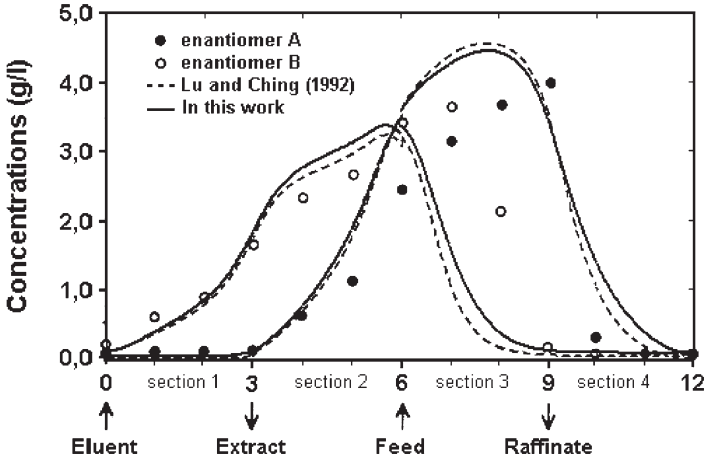

Figure 4. Instantaneous concentration profiles, in the half of the switch interval, of the enantiomers separation of the chiral epoxide in a SMB unit, in the cyclic steady state; (●) and (○) experimental points for the enantiomer less adsorbed (A) and more adsorbed (B), respectively (22); (- - -) numerical profiles obtained by Lu and Ching (21); and (—) numerical concentration profiles obtained in this work.

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transfer model and the existence of high concentration levels occurring in this section. Azevedo et al. (18) discuss that the LDF approximation may be as accurate as the bi-LDF, which offers a more realistic picture of the actual structure of the solid adsorbents, considering the mass transfer in macro and micropores, except for the microparticle diffusion control. The discrepancy can also be related with an inaccurate description of the adsorption equilibrium.

The computational program developed is used to examine the effect of the system configuration variation, i.e., the number of subsections in each section. The performance variables of process—purity and recovery—of the species in the raffinate and extract streams are considered when the cyclic steady state is reached. The values of the operating conditions and model parameters are those presented in Table 1, except for the configuration that is different for each simulation. The results can be visualized in Figs. 5 and 6, and in Table 2.

During the analysis of Figs. 5 and 6, two important points in the separation performance are verified when the SMB configuration is changed. Taking the configuration 3-3-3-3 as reference in these figures, in the SMB configurations on the right, the number of subsections in Sections 1 and 3 is larger than that in Sections 2 and 4. In Sections 1 and 3, the enantiomer with larger affinity with the adsorbent phase is desorbed and adsorbed, respectively. It is shown in Fig. 5 in these cases that the purity of the enantiomer with less affinity with the adsorbent,

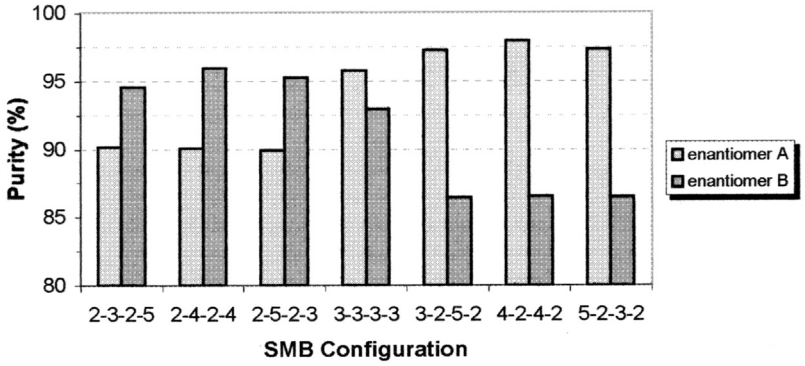

Figure 5. Purity of the enantiomers for the different configurations of the SMB unit with 12 sections.

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collected therefore in the raffinate, is larger than that collected in the extract. The recovery (Fig. 6), on the other way, is larger in the extract, in consequence to the purity obtained, i.e., a low purity of the more retained enantiomer means that there is a contamination for the less retained enantiomer in the extract. This consequently affects the recovery in the raffinate of this latter.

On the other hand, taking into account the unit configurations to the left of the reference configuration, the number of subsections in Sections 2 and 4 is larger than that in Sections 1 and 3. In Sections 2 and 4 the enantiomer with less affinity to the adsorbent phase is desorbed and adsorbed, respectively. Observing the purity values obtained for these configurations, in relation to more strongly

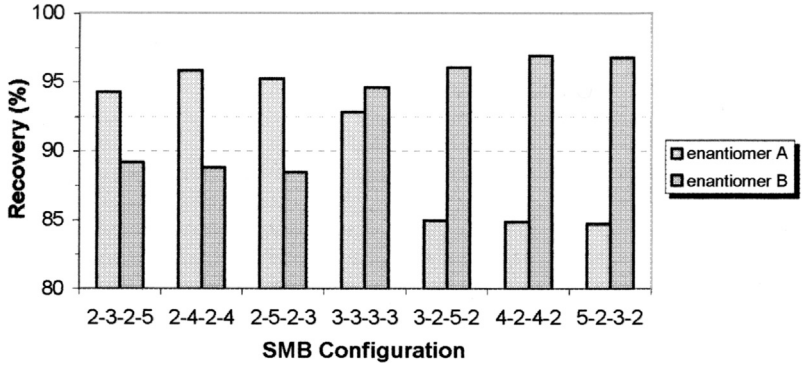

Figure 6. Recovery of the enantiomers for the different configurations of the SMB unit with 12 sections.

Table 2. Effect of Varying Bed Configuration on Purity of the Enantiomers in Their Enrichment Streams

	Purity (%)	
SMB Configuration	Raffinate	Extract
2 2 3 5	94.0	90.7
2 3 5 2	95.5	91.6
3 5 2 2	91.9	89.5
5 2 2 3	93.8	88.6
2 4 4 2	95.2	91.0
4 2 2 4	93.3	89.7

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adsorbed enantiomer, it is noticed that they are larger than that obtained for the other enantiomer collected in the raffinate. These facts can be related to the sections of the SMB unit performing adsorption and desorption functions of a certain species better and strictly, favoring the purification of a given species.

A comparison of the performance variables of the three configurations is made on the right and on the left of the configuration 3-3-3-3. On the right, there are configurations where Sections 1 and 3 are larger than the Sections 2 and 4, and the number of subsections in these two sections are altered. The purity values obtained for both species in the three configurations on the right are almost the same; the same behavior is also observed for the species recovery. This observation is verified with the configurations on the left of the configuration 3-3-3-3, in which occurs the variation of the number of subsections in Sections 2 and 4, maintaining the number of subsections in Sections 1 and 3. The purity and the recovery for the two enantiomers are slightly affected. The influence on the separation performance in the SMB unit is not so significant, when the number of subsections is increased or decreased in the sections where a certain species is adsorbed and desorbed, while the number of subsections is maintained in the sections whose functions are related to the other species.

Other examined configuration types are presented in Table 2, which shows the purity of the products. In Table 2, the unit configuration was altered in a sequential form, i.e., increasing or decreasing the number of subsections in consecutive sections (except for the two last configurations). As a result, it is also verified that the effect of this change of the configuration in the unit, regarding the separation performance, is small. It is worth mentioning that configurations where fractionation sections (Sections 2 and 3) are the largest, such as 2-3-5-2 and 2-4-4-2, allow obtaining higher purities for both enantiomers. For practical aims, the choice of the best configuration to be adopted in a separation process

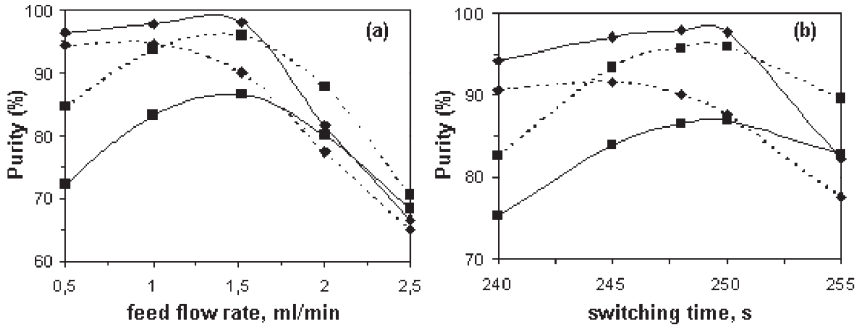

Figure 7. Effect of the operating parameters on the separation performance for two different SMB configurations. (a) Effect of the feed flow rate on product purity. (b) Effect of the switching time on product purity. (◆) enantiomer A; (■) enantiomer B; (—) configuration 2-4-2-4; (- - -) configuration 4-2-4-2 (based on the values shown in Table 1).

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will depend on the product purity requirements for a given species in the extract or/and raffinate streams.

Effects of the feed flow rate and switching time on the purity of the products for two different configurations are shown in Fig. 7. As known, the SMB performance is very sensitive to the operation conditions, where in the cases studied higher purities can be obtained only in a narrow range of values of feed flow rate as well as switching time.

As shown in Fig. 7, it is possible to obtain the optimal operating conditions for each configuration. Once the definition of a strict purity (or recovery) specification, and then the adequate configuration, has been determined, the choice of the best conditions can be performed, based on process simulation, supported by SMB package developed.

CONCLUSIONS

The resolution of the separation of (±)1a,2,7,7a-tetrahydro-3-methoxy-naphta-(2,3b)-oxirane enantiomers by SMB chromatography was simulated by the transient mathematical model. The numerical concentration profiles obtained in this work were compared with the experimental and numerical data presented in literature. Although the comparison of numerical results has shown a good concordance, the agreement with experimental concentration profiles has shown some scatter. The deviations could be caused by the negligence to the dead volume at both ends of the columns, the use of the LDF model and high concentrations in the Section 3.

The model, resolved numerically by the Method of Finite Volumes, has allowed obtaining the actual description of the SMB behavior in relation to the concentration profile of the involved species obtained along the operational time in the separation process of the enantiomers. The results obtained with a great number of subsections in the SMB unit are similar to TMB unit.

It was possible to study the influence of the configuration change of the subsections in the unit sections regarding the separation performance. It has been observed that this process parameter can alter the unit performance in the separation, allowing to obtain larger values of purity or recovery for a certain species, depending on the choice of the SMB configuration.

NOTATIONS

c_{ik}	fluid phase concentration of species i in subsection k, kg/m^3
D_{ak}	axial dispersion coefficient in the subsection k, m^2/sec
k_{T}	mass transfer coefficient, sec^{-1}
L	subsection length, m
q_{ik}	average adsorbed phase concentration of species i in subsection k, kg/m^3
q_{ik*}	adsorbed concentration of species i in subsection k in equilibrium with c_{ik}, kg/m^3
Pu	purity, dimensionless
Q	flow rate, m^3/sec
Re	recovery, dimensionless
v	interstitial fluid velocity in the subsection k, m/sec
t^*	switch time, sec
t	time, sec
z	axial coordinate, m

Greek Letters

ϵ	bed porosity, dimensionless

Subscripts and Superscripts

A	less retained enantiomer
B	more retained enantiomer
D	eluent
ex	extract
f	feed
i	chemical species
k	SMB subsections
ra	raffinate

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REFERENCES

1. Ruthven, D.M. *Principles of Adsorption and Adsorption Processes*; John Wiley: New York, 1984.
2. Ruthven, D.M.; Ching, C.B. Counter-Current and Simulated Counter-Current Adsorption Separation Processes. Chem. Eng. Sci. **1989**, *44* (5), 1011–1038.
3. Guest, D.W. Evaluation of Simulated Moving Bed Chromatography for Pharmaceutical Process Development. J. Chromatogr. A **1997**, *760*, 159–162.
4. Zhong, G.; Guiochon, G. Simulated Moving Bed Chromatography. Comparison Between the Behaviors Under Linear and Nonlinear Conditions. Chem. Eng. Sci. **1997**, *52* (23), 4403–4418.
5. Keller, G.E. II. Adsorption: Building upon a Solid Foundation. Chem. Eng. Prog. **1995**, *91*, 56.
6. Navarro, A.; Caruel, H.; Rigal, L.; Phemius, P. Continuous Chromatographic Separation Process: Simulated Moving Bed Allowing Simultaneous Withdrawal of Three Fractions. J. Chromatogr. A **1997**, *770*, 39–50.
7. Ching, C.B.; Ruthven, D.M. An Experimental Study of a Simulated Counter-Current Adsorption System—I. Isothermal Steady State Operation. Chem. Eng. Sci. **1985**, *40* (6), 877–885.
8. Azevedo, D.C.S.; Pais, L.S.; Rodrigues, A.E. Enantiomers Separation by SMB Chromatography: the Case of Non-Instantaneous Equilibrium at the Solid–Fluid Interface. J. Chromatogr. A **1999**, *865*, 187–200.
9. Storti, G.; Masi, M.; Carrà, S.; Morbidelli, M. Optimal Design of Multicomponent Countercurrent Adsorption Separation Processes Involving Nonlinear Equilibria. Chem. Eng. Sci. **1989**, *44* (6), 1329–1345.
10. Rodrigues, A.E.; Loureiro, J.M.; Lu, Z.P.; Pais, L.S. Modeling and Operation of a Simulated Moving Bed for the Separation of Optical Isomers. In *Fundamentals of Adsorption*; LeVan, M.D., Ed.; Kluwer Academic Publishers: Boston, MA, 1996.
11. Pais, L.S.; Loureiro, J.M.; Rodrigues, A.E. Separation of 1,1′-bi-2-naphthol Enantiomers by Continuous Chromatographic in Simulated Moving Bed. Chem. Eng. Sci. **1997**, *52* (2), 245–257.
12. Ching, C.B.; Ruthven, D.M.; Hidajat, K. Experimental Study of a Simulated Counter-Current Adsorption System—III. Sorbex Operation. Chem. Eng. Sci. **1985**, *40* (8), 1411–1417.
13. Pais, L.S.; Loureiro, J.M.; Rodrigues, A.E. Modeling, Simulation and Operation of a Simulated Moving Bed for Continuous Chromatographic Separation of 1,1′-bi-2-naphthol Enantiomers. J. Chromatogr. A **1997**, *769*, 25–35.

14. Silva, E.A.B. Modelagem e Simulação de uma Unidade de Leito Móvel Simulado. M.Sc. Thesis, UFSC-Florianópolis, Brazil.
15. Storti, G.; Baciocchi, R.; Mazzotti, M.; Morbidelli, M. Design of Optimal Operating Conditions of Simulated Moving Bed Adsorptive Separation Units. Ind. Eng. Chem. Res. **1995**, *34*, 288–301.
16. Ching, C.B.; Chu, K.H.; Hidajat, K.; Uddin, M.S. Comparative Study of Flow Schemes for a Simulated Countercurrent Adsorption Separation Process. A.I.Ch.E. J. **1992**, *38* (11), 1744–1750.
17. Azevedo, D.C.S.; Rodrigues, A.E. Design of a Simulated Moving Bed in the Presence of Mass-Transfer Resistances. A.I.Ch.E. J. **1999**, *45* (5), 956–966.
18. Azevedo, D.C.S.; Rodrigues, A.E. Bilinear Driving Force Approximation in the Modeling of a Simulated Moving Bed Using Bidisperse Adsorbents. Ind. Eng. Chem. Res. **1999**, *38* (9), 3519–3529.
19. Chu, K.H.; Hashim, M.A. Simulated Countercurrent Adsorption Processes: a Comparison of Modelling Strategies. Chem. Eng. J. **1995**, *56*, 59–65.
20. Pais, L.S.; Loureiro, J.M.; Rodrigues, A.E. Modeling Strategies for Enantiomers Separation by SMB Chromatographic. A.I.Ch.E. J. **1998**, *44*, 561–568.
21. Lu, Z.P.; Ching, C.B. Dynamics of Simulated Moving Bed Adsorption Separation Process. Sep. Sci. Technol. **1997**, *32* (12), 1993–2010.
22. Nicoud, R.M.; Fuchs, G.; Kusters, E.; Antia, F.; Reuille, R.; Schimid, E. *Preparative Scale Enantioseparation of a Chiral Epoxide—A Comparison of Liquid Chromatography and Simulated Moving Bed Adsorption Technology*; October 5–8 3rd International Symposium on Chiral Discrimination: Tuübingen, Germany, 1992; 5–8.
23. Rodrigues, A.E.; Pais, L.S.; Loureiro, J.M.; Lu, Z.P. Separation of Enantiomers of 1a,2,7,7a-tetrahydro-3methoxynaphtha-(2,3b)-oxirane by Liquid Chromatography: Laboratory-Scale Elution Chromatography and Modelling of Simulated Moving Bed. J. Chromatogr. A **1995**, *702*, 223–231.
24. Pais, L.S.; Loureiro, J.M.; Rodrigues, A.E. Separação de Enantiómeros de 1a,2,7,7a-tetrahidro-3-metoxinafta-(2,3b)-oxirano por Cromatografia Líquida em Leito Móvel Simulado, 1° Encontro Brasileiro sobre Adsorção, Fortaleza, Brazil, 1997.
25. Raithby, G.D. *Prediction of Dispersion by Surface Discharge, Basin Investigation and Modelling Section*; Canada Centre for Inland Waters: Burlington, Ontario, Canada, 1976.
26. Schneider, G.E.; Zedan, M. A Modified Strongly Implicit Procedure for the Numerical Solution of Field Problem. Numer. Heat Transfer **1981**, *4*, 1–19.

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